a corresponding spectral line based on data compiled in the spectral database (e.g., NIST).

Spectral peak: This term is used herein to refer to a measurement of the excitation of an emitter in a composition.

Spectrum: This term is used herein to refer to a plot showing intensity vs. mass-to-charge ratio in a particular chemical analysis of a composition.

Upper level population: This term is used herein to refer to the population of the upper energy level involved in an emission transition.

The advantages set forth above, and those made apparent from the foregoing description, are efficiently attained. Since certain changes may be made in the above construction without departing from the scope of the invention, it is intended that all matters contained in the foregoing description or shown in the accompanying drawings shall be interpreted as illustrative and not in a limiting sense.

It is also to be understood that the following claims are intended to cover all of the generic and specific features of the invention herein described, and all statements of the scope of the invention that, as a matter of language, might be said to fall therebetween.

What is claimed is:

1. One or more tangible non-transitory computer-readable media having computer-executable instructions for performing a method of running a software program on a computing device, the computing device operating under an operating system, the method including issuing instructions from the software program to analyze an analyte via atomic emission spectroscopy, the instructions comprising:

receiving a spectral database containing spectral information, said spectral information including spectral peak information and emitter information associated with said spectral peak information;

receiving an atomic emission spectrum including one or more spectral peaks associated with an emitter of said analyte, said spectrum being a multimodal probability distribution over a variable being wavelength of emitters;

identifying possible emitters associated with said one or more spectral peaks based on said spectral information in said spectral database, said identification based on a comparison of each individual peak of said one or more spectral peaks to said spectral information contained in said spectral database, wherein each of said possible emitters has a wavelength;

determining emission strength of said wavelength of said each possible emitter for said one or more spectral peaks, said emission strength associated with intensity of said each possible emitter of said one or more spectral peaks;

normalizing said emission strength of said each possible emitter to a probability range such that a sum of resulting probabilities of assignments of said each possible emitter of said one or more spectral peaks equals about 100% over a spectral range, said normalization of said one or more spectral peaks indicating said emission strength of said possible emitters, such that said emission strength of said each possible emitter is utilized as a probability for assignment of said each possible emitter with said wavelength of said each possible emitter being said variable for said multimodal probability distribution in order to determine probability of said assignment of said each possible emitter in said spectrum; and

automatically determining a level of confidence of identification of said each possible emitter based on said resulting probabilities of assignments of said possible emitters.

2. One or more tangible non-transitory computer-readable media as in claim **1**, further comprising:

said emission strength being selected from the group consisting of an upper level population or an oscillator strength of said possible emitters.

3. One or more tangible non-transitory computer-readable media as in claim **2**, further comprising:

said oscillator strength included in said spectral database.

4. One or more tangible non-transitory computer-readable media as in claim **1**, further comprising:

said one or more spectral peaks being a plurality of spectral peaks,

performing the foregoing steps to determine said level of confidence for assignment of each of said plurality of spectral peaks; and

performing an inference calculation to correct for inference and dependency between or among said plurality of spectral peaks.

5. One or more tangible non-transitory computer-readable media as in claim **1**, further comprising:

correcting for a background of said spectrum and extracting noise from said spectrum to facilitate said spectrum being said multimodal probabilistic distribution.

6. One or more tangible non-transitory computer-readable media as in claim **1**, wherein the step of normalizing said emission strength is performed by multiplying said emission strength by a value of the spectrum at a wavelength of said emitter.

7. One or more tangible non-transitory computer-readable media as in claim **1**, further comprising:

generating a profile of said spectrum based on said level of confidence calculated for said each possible emitter.

8. A computer-implemented method of automatically quantitatively determining a level of confidence for identification of an emitter represented by a spectral peak obtained via atomic emission spectroscopy, comprising:

receiving a spectral database containing spectral information, said spectral information including spectral peak information and emitter information associated with said spectral peak information;

receiving an atomic emission spectrum including one or more spectral peaks associated with an emitter of an analyte, said spectrum being a multimodal probability distribution over a variable being wavelength of emitters;

identifying possible emitters associated with said one or more spectral peaks based on said spectral information in said spectral database, said identification based on a comparison of each individual peak of said one or more spectral peaks to said spectral information contained in said spectral database, wherein each of said possible emitters has a wavelength;

determining emission strength of said wavelength of said each possible emitter for said one or more spectral peaks, said emission strength associated with intensity of said each possible emitter of said one or more spectral peaks;

normalizing said emission strength of said each possible emitter to a probability range such that a sum of resulting probabilities of assignments of said each possible emitter of said one or more spectral peaks equals about 100% over a spectral range, said normalization of said one or more spectral peaks indicating